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14. ABSTRACT					
This document is the final report on our research sponsored by AFOSR.					
inis document is the linal report on our research sponsored by AFOSR.					
The goal of our project remains: The design, analysis, and implementation					
of optimization tools to aid in making and documenting decisions involving					
trading off multiple objectives for mixed variable, generally constrained					
problems with no global smoothness assumptions.					
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From:

Charles Audet,

Charles.Audet@gerad.ca

John E. Dennis, Jr., dennis@rice.edu

Mark A. Abramson, Mark.A. Abramson@boeing.com

To: technicalreports@afosr.af.niil

Subject: Final report to Dr. Don Hearn

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Algorithms for Blackbox Optimization using Surrogate Functions

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Summary of accomplished work:

We produce algorithms and software to solve real problems. However, we are not interested in solving collaborators' problems with ad hoc methods; we are interested in using their real problems to motivate our main interest: the design and rigorous analysis of algorithms under hypotheses as close as possible to the context in which our algorithms will be used. This has led us to unique applications of nonsmooth nonconvex analysis techniques. This approach is now being used by other researchers in their methods for engineering design problems. We regard as one of our major career achievements the introduction of nonsmooth techniques to nonlinear simulation based design.

Two students completed their doctoral studies in summer 2008 under the supervision of Audet. Both their projects are directly tied to this research.

- Sebastien Le Digabel extended our black box optimization algorithm in three directions:
 - He coupled it in a generic way to the variable neighborhood search algorithm of Hansen et al., to globalize the method. This lead to a publication in *Journal of Global Optimization*.
 - He extended our derivative-free approach to higher dimensions, and he showed that we could tackle problems at least up to 500 variables. This lead to a publication in SIAM Journal on Optimization.
 - He replaced our default implementation in NOMAD by correcting two drawbacks of the previous method: the new method is deterministic, and avoids large cones of unexplored directions at every iteration. The paper is in its second round of review for SIAM Journal on Optimization.

Le Digabel's thesis was nominated for the best thesis in the Mathematics and Industrial Engineering department.

It is available at www.gerad.ca/Sebastien.Le.Digabel.

• Walid Zghal extended our algorithm to handle more than one objective function. His first project focused on the biobjective case, and it proposed and analyzed a new algorithm. It was published in SIAM Journal on Optimization. A second paper, submitted to Review of Quantitative Finance and Accounting, specializes this approach to optimal portfolio selection in finance. His last project couples our algorithm with the normal boundary intersection method of Das and Dennis, which was developed with support from and earlier AFOSR grant. His thesis can be downloaded from www.gerad.ca/Walid.Zghal.

During the last years we have pursued the development, theoretical analysis and practical applications, of direct search methods for black box optimization problems. In addition to the PhD projects described above, our main accomplishments include the following.

- We have proposed two alternatives to the drastic extreme barrier approach to constraints in which all infeasible points are rejected. The progressive barrier places a threshold on a constraint violation function, above which an infeasible trial point is discarded from consideration. Infeasible trial points under that threshold are investigated further. Then, as the algorithm proceeds, the threshold is reduced so that the iterates approach the feasible region. This paper uses concepts from the Clarke nonsmooth calculus to analyze the convergence, and will appear in SIAM Journal on Optimization. The second approach that we proposed starts by handling constraints by the progressive barrier, and as soon as a constraint is satisfied, it gets handled by the extreme barrier. Intensive testing of these approaches on three real engineering problems is performed in a paper provisionally accepted by Computational Optimization and Applications.
- In order to compare several algorithms designed to handle black box functions, Professor C. T. Kelley of North Carolina State University made public a series of nonlinear well location optimization problems that require the use of a flow solver to evaluate the objective function. We were coauthors with Kelley and others on a paper that published the numerical results for 6-8 different software packages, including our NOMAD. Our preliminary results show that NOMAD often improved the initial solution at a rate faster than the other methods, and often produced the best overall solution. This despite the fact that the problem has some quirky implementation details that alleviate the need for some important unique features of NOMAD, and indeed, penalize their use. This led to a publication in Advances in Water Resources.
- Many engineering optimization problems involve a special kind of discrete variable that can be represented by a number, but this representation has no utility. Such variables arise when a decision involves some situation like a choice from an unordered list of options. This has two implications: The standard approach of solving problems with continuous relaxations of discrete variables is not available, and the notion of local optimality must be defined through a user-specified set of neighboring points. We published a paper in Optimization Letters that extends previous work to the MADS class of algorithms, and that provides limit points that satisfy some appropriate necessary conditions

for local optimality for such problems.

- Aluminum is the second most used metal on Earth. Its production consists of three well-known steps: bauxite's extraction, alumina (Al₂O₃) separation from bauxite, and finally, alumina electrolysis. In the last step it is put into large baths of hot (960 °C) molten salts. These baths have an inside carbon lining, which must be replaced every 5 to 8 years, because they slowly degrade. This carbon lining and its attached refractories are called "spent potliners", and they are contaminated by fluoride, cyanide, and other hazardous materials. The MADS algorithm was used to optimize a recent spent potliner treatment process. This resulted in a 37% reduction of the treatment cost. A difficult aspect of this problem, which NOMAD is designed to handle, is that the model failed to return a value 43% of the times it was called. This led to a publication in Optimization and Engineering.
- Our NOMAD C++ software was entirely revised. The previous version had reached its potential limit, which was not surprising, since its fundamental design dated back from 2000. The new version is now much closer to the algorithmic descriptions appearing in the peer-reviewed papers. NOMAD can now solve general nonlinearly constrained optimization problems using the method. The software is available at www.gerad.ca/nomad.
- Several papers have appeared in top peer reviewed journals. Our papers combine theoretical results, analysis of the limitations of GPS and numerical results on some real engineering problems. Several others are submitted, and we expect them to be accepted in a near future.

We continue our close collaboration with Boeing, ExxonMobil, and GM. New collaborations were initiated with IREQ on optimal positioning of GMON snow sensors to estimate water income at hydroelectrical dams, with LANL for rapid quantitative object reconstruction from a single x-ray radiograph, and with UCSD for optimal design of artificial conduits for surgical correction of pediatric cardiology problems. The first result of this project is expected to be implanted in a patient this fall.

Personnel Supported:

Faculty: Charles Audet, John Dennis and Mark Abramson Research Staff: Gilles Couture and Sébastien Le Digabel Students: Walid Zghal, Sébastien Le Digabel, Kien Cong Dang,

Summer interns: Mohammed Sylla.

Archival publications published during reporting period:

Published:

- 1. M.A. Abramson, C. Audet, J.W. Chrissis, and J.G. Walston. Mesh adaptive direct search algorithms for mixed variable optimization. *Optimization Letters*, 3(1):35–47, 2009.
- 2. C. Audet, P. Hansen, and F. Messinc. Isoperimetric polygons of maximum width. *Discrete and Computational Geometry*, 41(1):45–60, 2009.
- 3. C. Audet, P. Hansen, and F. Messine. Simple polygons of maximum perimeter contained in a disk of radius onc. *Discrete and Computational Geometry*, 41(2):208–215, 2009.
- 4. Charles Audet, J. E. Dennis, and Sébastien Le Digabel. Parallel space decomposition of the mesh adaptive direct search algorithm. *SIAM Journal on Optimization*, 19(3):1150–1170, 2008.
- M.A. Abramson, T.J. Asaki, J.E. Dennis Jr., K. R. O'Reilly, and R. L. Pingel. Quantitative object reconstruction using Abel transform x-ray tomography and mixed variable optimization SIAM Journal on Imaging Sciences, 1(3):322–342, 2008.
- M.A. Abramson, O.A. Brezhneva, J.E. Dennis Jr., and R.L. Pingel. Pattern search in the presence of degenerate linear constraints. *Optimization Methods and Software*, 23(3):297–319, 2008.
- J.A. Beal, A. Shukla, O.A. Brezhneva, and M.A. Abramson. Optimal sensor placement for enhancing sensitivity to change in stiffness for structural health monitoring *Optimization and Engineering*, 9(2):119– 142, 2008.

- 8. K.R. Fowler, J.P. Reese, C.E. Kees, J.E. Dennis Jr., C.T. Kelley, C.T. Miller, C. Audet, A.J. Booker, G. Couture, R.W. Darwin, M.W. Farthing, D.E. Finkel, J.M. Gablonsky, G. Gray, and T.G. Kolda. Comparison of derivative-free optimization methods for groundwater supply and hydraulic capture community problems. *Advances in Water Resources*, 31(5):743–757, 2008.
- 9. A. L. Custódio, J. E. Dennis Jr. and L. N. Vicente. Using simplex gradients of nonsmooth functions in direct search methods. *IMA Journal of Numerical Analysis* 28: 770–784, 2008.
- C. Audet, P. Hansen, and F. Messine. Ranking small regular polygons by area and by perimeter. *Discrete Analysis and Operations Research*, 15(3):65-73, 2008.
- 11. C. Audet, P. Hansen, A. Karam, C. Ng, and S. Perron. Exact l_2 -norm plane separation. *Optimization Letters*, 2(4):483–495, 2008.
- 12. C. Audet, V. Béchard, and S. Le Digabel. Nonsmooth optimization through mesh adaptive direct search and variable neighborhood search. *Journal of Global Optimization*, 41(2):299–318, 2008.
- C.Audet, V. Béchard, and J. Chaouki. Spent potliner treatment process optimization using a mads algorithm. Optimization and Engineering, 9(2):143-160, 2008.
- 14. C. Audet, A. Custódio, and J. E. Dennis, Jr. Erratum: Mesh adaptive direct search algorithms for constrained optimization,. *SIAM Journal on Optimization*, 18(4):1501–1503, 2008.
- 15. C. Audet, G. Savard, and W. Zghal. Multiobjective optimization through a series of single-objective formulations. *SIAM Journal on Optimization*, 19(1):188–210, 2008.
- 16. M.A. Abramson, C. Audet, and J. E. Dennis, Jr. Filter pattern search algorithms for mixed variable constrained optimization problems. *Pacific Journal on Optimization*, 3(3):477–500, 2007.
- 17. C. Audet, G. Savard, and W. Zghal. New branch-and-cut algorithm for bilevel linear programming. *Journal of Optimization Theory and Applications*, 134(2):353–370, 2007.
- 18. C. Audet, P. Hansen, and F. Messine. Extremal problems for convex polygons. *Journal of Global Optimization*, 38(2):163–179, 2007.
- 19. C. Audet, J. Haddad, and G. Savard. Disjunctive cuts for continuous linear bilevel programming. *Optimization Letters*, 1(3):259–267, 2007.

20. A. L. Marsden, M. Wang and J. E. Dennis, Jr., and P. Moin. Trailing-edge noise reduction using derivative-free optimization and large-eddy simulation. *Journal of Fluid Mechanics*, 572: 13–36, 2007

Accepted for Publication:

- 1. C. Audet, S. Belhaïza, and P. Hansen. A new sequence form approach for the enumeration of all extreme Nash equilibria for extensive form games. To appear in *International Game Theory Review*, 2009.
- 2. C. Audet, P. Hansen, and F. Messine. Extremal problems for convex polygons an update. To appear in *Fields Institute Communications*, 2009.
- 3. C. Audet and J. E. Dennis, Jr. A MADS algorithm with a progressive barrier for derivative-free nonlinear programming. To appear in *SIAM Journal on Optimization*, 2009.
- N.P. Sherman, J.P. Kharoufeh, and M.A. Abramson. An M/G/1 retrial queue with unreliable server for streaming multimedia applications. To appear in *Probability in the Engineering and Informational Sciences*, 2009.
- 5. T.A. Sriver, J.W. Chrissis, and M.A. Abramson (2009). Pattern search ranking and selection algorithms for mixed variable simulation-based optimization. To appear in *European Journal of Operational Research*, 2009

Submitted for Publication:

- M.A. Abramson, L. Frimannslund, T. Steihaug. A subclass of generating set search with convergence to second-order stationary points Technical Report, Rice CAAM-TR, 2009.
- M.A. Abramson, T.J. Asaki, J.E. Dennis Jr., R. Magallanez, and M.J. Sottile. Solving computationally expensive optimization problems with CPU time-correlated functions Technical Report, Rice CAAM-TR08-06, 2008.
- C. Audet, J. E. Dennis, Jr., and S. Le Digabel. Globalization strategies for mesh adaptive direct search. Les Cahiers du GERAD G-2008-74, GERAD, November 2008.

- 4. C. Audet, A. Guillou, P. Hansen, S. Perron, and F. Messine. The small hexagon and heptagon with maximum sum of distances between vertices. Technical Report Les Cahiers du GERAD G-2008-20, 2008.
- 5. C. Audet, M.A. Abramson, J.E. Dennis, and S. Le Digabel. Orthomads: A deterministic mads instance with orthogonal directions. Technical Report Les Cahiers du GERAD G-2008-15, 2008.
- C. Audet, P. Hansen, and S. Perron. Remarks on solutions to a nonconvex quadratic programming test problem. Technical Report Les Cahiers du GERAD G-2007-88, 2008.
- C. Audet, S. Belhaïza, and P. Hansen. Perfect and proper refinements of all extreme nash equilibria for bimatrix games. Technical Report Les Cahiers du GERAD G-2007-85, 2007.
- 8. C. Audet, G. Savard, and W. Zghal. A new multi-objective approach for the portfolio selection problem with skewness. Technical Report Les Cahiers du GERAD G-2007-86, 2007.
- S.F. Arroyo, E.J. Cramer, J.E. Dennis, Jr. and P.D. Frank. Comparing problem formulations for coupled sets of components. Technical Report, Rice CAAM-TR07-16, 2007.
- 10. J.C. Meza, A. Garcia-Lekue, M.A. Abramson, and J.E. Dennis Jr.. Surface structure determination of nanostructures using a mesh adaptive optimization method, 2007.

Public Presentations:

Charles Audet – Invited plenary talks

- "Derivative-Free Optimization: Theory and Practice". SIOPT annual meeting; Boston, USA, May 2008.
- "Optimal placement of tsunami warning buoys using mesh adaptive direct searches". *Optimization Days*; Montréal, Canada, May 2007.
- "Mesh Adaptive Direct Searches for Constrained Optimization". Optimization 2007; Porto, Portugal; July 2007.

J. E. Dennis

Over the past 5 years, John Dennis has given over 100 hour lectures at meetings, universities, and government and industrial labs.

Mark A. Abramson

- Guest lecturer for 5-hour optimization shortcourse at the LANL Data Sciences Summer School.
- Gave 3-hour Introduction to Applied Optimization tutorial at the 1st AIAA Multidisciplinary Design Optimization Specialist Conference, as part of the 46th AIAA/ASME/ASCE/AHS/ASC Structures, Structural Dynamics, and Materials Conference

Changes in research objectives: None.

The goal of our project remains: The design, analysis, and implementation of optimization tools to aid in making and documenting decisions involving trading off multiple objectives for mixed variable, generally constrained problems with no global smoothness assumptions.

Change in AFOSR program manager, if any: None

Extensions granted or milestones slipped, if any: None

New discoveries, inventions, or patent: None